



chain nodes :

21 22 23 24 25 26 27 28 29 30 31 32 33 35 37 38 39 44 45 46

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

4-21 6-31 8-22 13-17 14-30 17-26 18-25 18-29 19-24 19-28 20-23 21-22 21-32 23-27  
24-45 25-46 27-44

ring bonds :

1-2 1-6 2-3 2-13 3-4 3-15 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15  
16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

2-13 3-15 4-21 13-14 13-17 14-15 16-17 16-20 17-18 18-19 18-25 19-20 19-24

exact bonds :

6-31 8-22 14-30 17-26 18-29 19-28 20-23 21-22 21-32 23-27 24-45 25-46 27-44

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:F, I, CHO, NO2, S, CH3, OH, EtO, CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS  
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS  
31:CLASS 32:CLASS 33:CLASS 34:Atom 35:CLASS 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:Atom  
41:Atom 42:Atom 44:CLASS 45:CLASS 46:CLASS